given by multiplication by the lattice $l(\mathbf{r})$. The corresponding convolution in reciprocal space gives the same contribution to all Bragg reflections (Fig. 4.2.3.2*e*).

(ii) There is no perfect lattice geometry. In this case a continuous Patterson function results. Fourier transformation yields an influence which is now restricted primarily to the reflection 000, *i.e.* to the low-angle diffraction range.

Figs. 4.2.3.2(*e*), (*f*) show the different diffraction patterns of the diffuse scattering which is concentrated around the Bragg maxima. Although the discussion of the diffuse scattering was restricted to the case of identical domains, the introduction of a distribution of domain sizes does not influence the diffraction pattern essentially, as long as the fluctuation of sizes is small compared with the average volume of domain sizes and no strong correlation exists between domains of any size (size-independent random distribution).

The complete qualitative discussion of the diffraction pattern may be made by investigating the Fourier transform of (4.2.3.21*a*):

$$[L(\mathbf{H}) * T(\mathbf{H})]|\Delta F(\mathbf{H})|^2|D(\mathbf{H})|^2. \qquad (4.2.3.21b)$$

The first factor in (4.2.3.21*b*) describes the particle-size effect of a domain containing the influence of a surrounding strain field and the new structure of the domains precipitated from the bulk. $D(\mathbf{H})$ has its characteristic variation near the Bragg peaks (Figs. 4.2.3.2*e*, *f*), and is less important in between. For structure determination of domains, intensities near the Bragg peaks should be avoided. Note that equation (4.2.3.21*b*) may be used for measurements applying anomalous scattering in both the centric and the acentric case.

Solution of the diffraction problem. In equation (4.2.3.21*b*) $\Delta F(\mathbf{H})$ is replaced by its average

$$\langle \Delta F(\mathbf{H})\rangle = \sum_{\mu} p_{\mu} \Delta F_{\mu}(\mathbf{H}),$$

where p_{μ} represents the *a priori* probability of a domain of type μ. This replacement becomes increasingly important if small clusters (domains) have to be considered. Applications of the formulae to Guinier–Preston zones are given by Guinier (1942) and Gerold (1954); a similar application to clusters of vacancies in spinels with an excess in Al_2O_3 was outlined by Jagodzinski & Haefner (1967).

Although refinement procedures are possible in principle, the number of parameters entering the diffraction problem becomes increasingly large if more clusters or domains (different sizes) have to be introduced. Another difficulty results from the large number of diffraction data which must be collected to perform a reliable structure determination. There is no need to calculate the first two terms in equation (4.2.3.20*c*) which do contribute to the sharp Bragg peaks only, because their intensity is simply described by the averaged structure factor $|\langle F(\mathbf{H})\rangle|^2$. These terms may therefore be replaced by

$$|L(\mathbf{H})|^2|\langle F(\mathbf{H})\rangle|^2$$

with

$$|\langle F(\mathbf{H})\rangle|^2 = \left|\sum_{\mu} p_{\mu} F_{\mu}(\mathbf{H})\right|^2 \qquad (4.2.3.21c)$$

where p_{μ} is the *a priori* probability of the structure factor $F_{\mu}(\mathbf{H})$. It should be emphasized here that (4.2.3.21*c*) is independent of the distribution function $d(\mathbf{r})$, or its Fourier transform $D(\mathbf{H})$.

(2) *Periodic lamellar domains*

Here $d(\mathbf{r})$ is one-dimensional, and can easily be calculated: a periodic array of two types of lamellae having the same basic lattice $l(\mathbf{r})$, but a different structure, is shown in Fig. 4.2.3.3. The size of the two types of lamellae may be different. The structure of the first domain type is given by a convolution with $F_1(\mathbf{r})$ (Fig. 4.2.3.3*a*) and that of the second domain type by $F_2(\mathbf{r})$ (Fig. 4.2.3.3*b*). Introducing $\langle F(\mathbf{r})\rangle$ and $\Delta F(\mathbf{r})$, the structure in real space is described by:

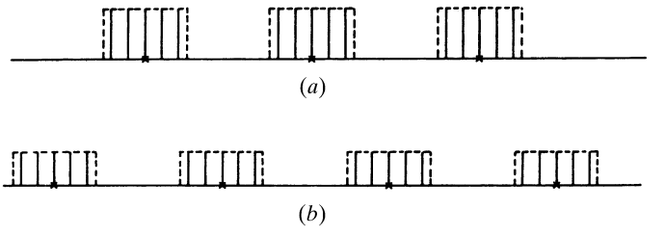

Fig. 4.2.3.3. Periodic array of domains consisting of two different atoms, represented by different heights. (*a*) Distribution of domain type 1, (*b*) distribution of domain type 2.

$$\begin{aligned}&[l(\mathbf{r})b_1(\mathbf{r})] * d(\mathbf{r}) * F_1(\mathbf{r}) + [l(\mathbf{r})b_2(\mathbf{r})] * d(\mathbf{r}) * F_2(\mathbf{r})\\ &\quad = \{[l(\mathbf{r})b_1(\mathbf{r}) + l(\mathbf{r})b_2(\mathbf{r})] * d(\mathbf{r})\} * \langle F(\mathbf{r})\rangle\\ &\qquad + [l(\mathbf{r})b_1(\mathbf{r}) - l(\mathbf{r})b_2(\mathbf{r})] * d(\mathbf{r}) * \Delta F(\mathbf{r}). \qquad (4.2.3.22a)\end{aligned}$$

Obviously the first term in curly brackets in equation (4.2.3.22*a*) is no more than $l(\mathbf{r})$ itself and $d(\mathbf{r})$ is strictly periodic. $b_1(\mathbf{r})$ and $b_2(\mathbf{r})$ are box functions, mutually displaced by $\pm(n_1 + n_2)/2$ unit cells in the $\mathbf{c}$ direction [n_1, n_2 are the numbers of cells covered by $b_1(\mathbf{r})$ and $b_2(\mathbf{r})$, respectively].

Fourier transformation of equation (4.2.3.22*a*) yields

$$L(\mathbf{H})\langle F(\mathbf{H})\rangle + \{L(\mathbf{H}) * [B_1(\mathbf{H}) - B_2(\mathbf{H})]\}D(\mathbf{H})\Delta F(\mathbf{H}). \qquad (4.2.3.22b)$$

The first term in equation (4.2.3.22*b*) gives the normal sharp reflections of the average structure, while the second describes superlattice reflections [sublattice $L_s(\mathbf{H}) = D(\mathbf{H})$ in reciprocal space], multiplied by $\Delta F(\mathbf{H})$ and another 'structure factor' generated by the convolution of the reciprocal lattice $L(\mathbf{h})$ with $[B_1(\mathbf{H}) - B_2(\mathbf{H})]$ (*cf.* Fig. 4.2.3.3*b*). Since the centres of $b_1(\mathbf{r})$ and $b_2(\mathbf{r})$ are mutually displaced, the expression in square brackets includes extinctions if $b_1(\mathbf{r})$ and $b_2(\mathbf{r})$ represent boxes equal in size. These extinctions are discussed below. It should be pointed out that $L_s(\mathbf{H})$ and its Fourier transform $l_s(\mathbf{r})$ are commensurate with the basic lattice, as long as no change of the translation vector at the interface of the lamellae occurs. Obviously, $L_s(\mathbf{H})$ becomes incommensurate in the general case of a slightly distorted interface. Considerations of this kind play an important role in the discussion of modulated structures.

No assumption has been made so far for the position of the interface. This point is meaningless only in the case of a strictly periodic array of domains (no diffuse scattering). Therefore it seems to be convenient to introduce two basic vectors parallel to the interface in real space which demand a new reciprocal vector perpendicular to them defined by $(\mathbf{a}' \times \mathbf{b}')/V'$, where $\mathbf{a}'$, $\mathbf{b}'$ are the new basic vectors and V' is the volume of the supercell. As long as the new basic vectors are commensurate with the original lattice, the direction of the new reciprocal vector $\mathbf{c}'^*$, perpendicular to $\mathbf{a}'$, $\mathbf{b}'$, passes through the Bragg points of the original reciprocal lattice and the reciprocal lattice of the superlattice remains commensurate as long as V' is a multiple of V ($V' = mV$, $m =$ integer). Since the direction of $\mathbf{c}$ is arbitrary to some extent, there is no clear rule about the assignment of superlattice reflections to the original Bragg peaks. This problem becomes very important if extinction rules of the basic lattice and the superlattice have to be described together.

references